Electronic, Optical, and Vibrational Properties of Bridged Dithienylethylene-Based NLO Chromophores

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Résumé en anglais	The vibrational, optical, and nonlinear optical (NLO) properties of a series of push?pull chromophores built around dithienylethylene-based π-conjugating spacers have been investigated by UV?vis, IR, and Raman spectroscopies and electric field-induced second harmonic generation (EFISH) measurements. The effects of the strength of the acceptor group on the molecular electronic properties of these conjugated NLO chromophores have been addressed. The magnitude of the intramolecular charge transfer has been tested as a function of the acceptor strength and of the bridging of the spacer. Density functional theory (DFT) calculations have been performed to help the assignment of the main electronic and vibrational features of the NLO chromophores and to derive useful information about their molecular structures. EFISH measurements show that push?pull systems that contain strong electron-acceptor groups connected via a rigidified dithienylene spacer exhibit large values of ??0. Theoretical NLO calculations are in excellent agreement with experimental results. The geometrical and electronic properties calculated in solution reveal that chromophores become highly polarized as the dielectric constant of the solvent increases. The spectroscopic properties/structure relationships agree with the observation that ?0 increases upon the covalent bridging of the spacer and with the increase of the acceptor strength.
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